Automatic Mass Spectral Deconvolution and Identification Software (AMDIS)

NIST has developed a software tool that allows users to identify a single component in a complex mixture. The disentanglement of the multiple signatures is called deconvolution and is accomplished by an ***Automatic Mass Spectral Deconvolution and Identification Software*** *(AMDIS) using a series of algorithms developed at NIST. The initial work was funded by the Defense Department in order to aid in the compliance with the Chemical Weapons Convention. The broader utility of the tool for analysis of complex mixtures (such as surface waters for pollutants, food for contamination, and complex fluids for medical applications) is only now being realized.*

G. Mallard and O. Toropov (Div. 838)

The problems of establishing chemical identity for trace species in complex matrices breaks down into two distinct pieces – isolating a single species and then analyzing the species so isolated. The tool of choice for many such complex matrices is the Gas Chromatograph coupled to the Mass Spectrometer. The data needed for identification of the species by mass spectrometry and NIST's role in providing such data is discussed elsewhere. The problem addressed here is extraction of the data for a single species. As mixtures become more complex or the concentration of a component decreases, the chromatographic process can not fully separate the component, and thus there are often multiple chemicals coming out "together" so that the mass spectral signatures are not clean enough to allow identification. Deconvolution, or the separation of multiple signatures, is accomplished by AMDIS using a series of algorithms developed at NIST.

The fundamental algorithms that make up AMDIS are very stable and only minor changes have been needed. However, AMDIS has evolved to handle new instruments, to better couple to instrumentation software and to deal with types of analyses for which it was not originally designed. These efforts have been coordinated with a number of instrumentation companies to make the use of AMDIS easier for customers. In addition, we have been working directly with laboratories that are developing tools to respond to possible terrorism events where very large numbers of samples will need to be analyzed at possibly very sensitive levels. This latter effort has been the focus of the last year. AMDIS has been used to reduce the noise in reference spectra taken for the analysis of pesticides, toxins, poisons, and industrial chemicals. The effect of acquiring improved data of this type is to provide more sensitivity for the analysis of these chemicals without a corresponding increase in the risk of false positive identification.

The release of AMDIS 2.64 occurred in December 2005. During the year a major effort was devoted to developing libraries that could be of use to the laboratory emergency response networks. We directly worked with the FDA's Forensic Chemistry Center in developing these libraries both from their data and the data from the FDA Pesticide Residue Laboratory in Seattle, WA. Experimental data from both of these libraries, which had been analyzed using conventional analysis techniques, was reanalyzed using AMDIS. This reanalysis automatically provided the retention index data as well as substantially better spectra. The data from the two laboratories as well as data on chemical weapons from the Organization for the Prohibition of Chemical Weapons database was combined with additional data from the NIST mass spectral library to create a library of toxic industrial chemicals, pesticides and chemical weapon related compounds that was provided to a number of state laboratories as part of a training conducted jointly by personnel from NIST and the FDA Forensic Chemistry Center in August 2006. Work is ongoing on improvements in the database.

AMDIS provides the first broadly available method for automating GC/MS analysis. With AMDIS an analyst can find, with high confidence, components in complex mixtures that would otherwise be missed as well as having greater confidence in all analytical results.

The productivity of analysts in the laboratory is significantly increased using AMDIS since the first pass analysis of the data is in minutes – without direct intervention, rather than hours – with full involvement of the analyst. AMDIS can also aid in providing statistically valid confidence measures for analysis.

AMDIS usage is steadily increasing. It is used as part of the proficiency exams for laboratories world wide which participate in the analysis for compliance with the Chemical Weapons Convention. Increasingly it is being used for metabolite studies in complex matrices such a whole plant and whole cell analysis. Finally, the adoption of AMDIS

as a part of the new DRS system of Agilent has meant that a far larger number of users will use it.

Publications and Presentations:

Mallard, W.G., ***"Extending AMDIS – Interactions with Instrument Software, Concentration Calculations and Increased Sensitivity"***, Agilent Technologies, Wilmington, DL, November 17, 2005.

Mallard, W.G., ***"FERN GC-MS Chemistry Training Course LB508"***, FDA Forensic Chemistry Center, Cincinnati, OH, August 15-17, 2006.

Future Plans: Specific changes in AMDIS are driven by the user community. Minor modifications in the algorithm to take into account varying scan ranges as are often used in the instrumentation, improved access to the algorithm using the DLL (dynamic link library) in order to facilitate the use by instrument companies within their own data systems have been made in the past year.

The use of AMDIS to aid in the development of specific libraries for problems of national interest has become an increasing part of the effort associated with AMDIS. These library developments are coupled to specific protocols for analysis. In addition, training courses in the use of AMIDS, again tied to specific protocols for analysis will be important parts of the future efforts to make AMDIS more widely used.